2-Methyl-p-benzoquinone
553-97-9 | DTXSID8060290

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 7.75e-01

Global applicability domain: Inside

Local applicability domain index: 6.53e-01

Confidence level: 6.59e-01

Nearest Neighbors from the Training Set

Image not found
2-Methyl-p-benzoquinone
Measured: 0.72
Predicted: 7.75e-01

Image not found
1,4-Benzoquinone
Measured: 0.2
Predicted: 4.89e-01

Image not found
2,5-Cyclohexadiene-1,4-dione,
2,5-dimethyl-
Measured: 1.28
Predicted: 1.26

Image not found
2,6-Dimethyl-1,4-benzoquinone
Measured: 1.22
Predicted: 1.25

Image not found
2,4,6-Cycloheptatrien-1-one, 3-
hydroxy-
Measured: 0.81
Predicted: 1.06